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**APPENDIX A**  
**ROBUST SUMMARIES**

# I U C L I D

## Data Set

**Existing Chemical** : ID: 4083-64-1  
**CAS No.** : 4083-64-1  
**EINECS Name** : p-toluenesulphonyl isocyanate  
**EC No.** : 223-810-8  
**Molecular Formula** : C<sub>8</sub>H<sub>7</sub>NO<sub>3</sub>S

**Producer related part**  
**Company** : Epona Associates, LLC  
**Creation date** : 09.06.2003

**Substance related part**  
**Company** : Epona Associates, LLC  
**Creation date** : 09.06.2003

**Status** :  
**Memo** : ISOCHEM Inc.

**Printing date** : 01.06.2004  
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**Date of last update** : 01.06.2004

**Number of pages** : 7

**Chapter (profile)** : Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2

**Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4  
**Flags (profile)** : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 2. Physico-Chemical Data

Id 4083-64-1

Date 01.06.2004

### 2.1 MELTING POINT

Value : = -2 °C  
Sublimation :  
Method :  
Year : 2002  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : Freezing Point  
Source : Epona Associates, LLC  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
09.06.2003

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### 2.2 BOILING POINT

Value : = 144 °C at 1333 hPa  
Decomposition :  
Method :  
Year : 2002  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : Pressure 10 mm Hg  
Source : Epona Associates, LLC  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
01.06.2004

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### 2.4 VAPOUR PRESSURE

Value : = 1.33 hPa at 100 °C  
Decomposition :  
Method :  
Year : 2002  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Result : 1 mm Hg @ 100 deg C  
Source : Epona Associates, LLC  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
01.06.2004

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### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water  
Log pow : = .82 at °C  
pH value :  
Method :  
Year : 1979  
GLP : no data  
Test substance : other TS

## 2. Physico-Chemical Data

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**Remark** : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3).

**Source** : Epona Associates, LLC

**Test substance** : CAS Registry Number: 70-55-3  
Chemical Name: P-TOLUENESULFONAMIDE  
Synonyms: 4-METHYLBENZENESULFONAMIDE  
Molecular Formula: C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>S  
Molecular Weight: 171.22

**Reliability** : (2) valid with restrictions

**Flag** : Critical study for SIDS endpoint

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### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water

**Value** : = 1318 mg/l at 25 °C

**pH value** :

**concentration** : at °C

**Temperature effects** :

**Examine different pol.** :

**pKa** : at 25 °C

**Description** :

**Stable** : no

**Deg. product** :

**Method** : other: estimated

**Year** : 2004

**GLP** : no

**Test substance** : as prescribed by 1.1 - 1.4

**Deg. products** : 70-55-3 200-741-1 toluene-4-sulphonamide

**Remark** : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3).

**Result** : WSKOW v1.41 Results  
Log Kow (estimated) : 2.34  
Log Kow (experimental): not available from database  
Log Kow used by Water solubility estimates: 2.34

Equation Used to Make Water Sol estimate:  
 $\text{Log S (mol/L)} = 0.693 - 0.96 \log \text{Kow} - 0.0092(\text{Tm} - 25) - 0.00314 \text{ MW} + \text{Correction}$

Melting Pt (Tm) = -2.00 deg C (Use Tm = 25 for all liquids)

Correction(s):      Value  
-----  
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -2.175  
Water Solubility at 25 deg C (mg/L): 1318

**Source** : Epona Associates, LLC

**Test condition** : log Kow used: 2.34 (estimated)  
no-melting pt equation used

**Reliability** : (2) valid with restrictions

**Flag** : Critical study for SIDS endpoint

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### 3. Environmental Fate and Pathways

Id 4083-64-1

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#### 3.1.1 PHOTODEGRADATION

Type : air  
Light source :  
Light spectrum : nm  
Relative intensity : based on intensity of sunlight  
**DIRECT PHOTOLYSIS**  
Half-life t<sub>1/2</sub> : ca. 8.8 day(s)  
Degradation : % after  
Quantum yield :  
**INDIRECT PHOTOLYSIS**  
Sensitizer :  
Conc. of sensitizer :  
Rate constant : = .000000000000122 cm<sup>3</sup>/(molecule\*sec)  
Degradation : % after  
Deg. product : not measured  
Method : other (calculated)  
Year : 2004  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4

**Result** : SUMMARY (AOP v1.91): HYDROXYL RADICALS  
Hydrogen Abstraction = 0.1360 E-12 cm<sup>3</sup>/molecule-sec  
Reaction with N, S and -OH = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
\*\*Addition to Aromatic Rings = 1.0883 E-12 cm<sup>3</sup>/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm<sup>3</sup>/molecule-sec  
  
OVERALL OH Rate Constant = 1.2243 E-12 cm<sup>3</sup>/molecule-sec  
HALF-LIFE = 8.737 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
HALF-LIFE = 104.839 Hrs  
\*\* Designates Estimation(s) Using ASSUMED Value(s)

SUMMARY (AOP v1.91): OZONE REACTION  
  
\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
(ONLY Olefins and Acetylenes are Estimated)

Source : Epona Associates, LLC  
Test substance : SMILES : O=C=NS(=O)(=O)c(ccc(c1)C)c1  
CHEM : Benzenesulfonyl isocyanate, 4-methyl-  
MOL FOR: C8 H7 N1 O3 S1  
MOL WT : 197.21

Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
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#### 3.1.2 STABILITY IN WATER

Type : abiotic  
t<sub>1/2</sub> pH4 : < 10 minute(s) at 25 °C  
t<sub>1/2</sub> pH7 : < 10 minute(s) at 25 °C  
t<sub>1/2</sub> pH9 : < 10 minute(s) at 25 °C  
Deg. product :  
Method : other  
Year : 2004  
GLP : no

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**Test substance** : as prescribed by 1.1 - 1.4  
**Deg. products** : 70-55-3 200-741-1 toluene-4-sulphonamide

**Result** : HYDROWIN Program (v1.67) Results:  
=====

Compound has an ISOCYANATE group; C=O located at SMILES atom #:  
2

\*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

Even at low pH, the hydrolysis rate is very fast:  $t_{1/2} < 10$  minutes.

**Source** : Epona Associates, LLC  
**Test substance** : SMILES : O=C=NS(=O)(=O)c(ccc(c1)C)c1  
CHEM : Benzenesulfonyl isocyanate, 4-methyl-  
MOL FOR: C8 H7 N1 O3 S1  
MOL WT : 197.21

**Reliability** : (2) valid with restrictions  
**Flag** : Critical study for SIDS endpoint  
02.04.2004 (5)

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

**Type** : fugacity model level III  
**Media** :  
**Air** : % (Fugacity Model Level I)  
**Water** : % (Fugacity Model Level I)  
**Soil** : % (Fugacity Model Level I)  
**Biota** : % (Fugacity Model Level II/III)  
**Soil** : % (Fugacity Model Level II/III)  
**Method** : other: estimated  
**Year** : 2004

**Remark** : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). PTSI is not likely to be found in the environment.

**Result** : Level III Fugacity Model (Full-Output):  
=====

Chem Name : Benzenesulfonyl isocyanate, 4-methyl-  
Molecular Wt: 197.21  
Henry's LC : 5.69e-005 atm-m<sup>3</sup>/mole (Henrywin program)  
Vapor Press : 5.29 mm Hg (Mppbwin program)  
Log Kow : 2.34 (Kowwin program)  
Soil Koc : 89.7 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	6.04	210	1000
Water	31.3	900	1000
Soil	62.5	900	1000
Sediment	0.174	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.22e-010	326	986	10.9	32.9
Water	7.36e-010	393	510	13.1	17
Soil	6.66e-009	785	0	26.2	0
Sediment	6.5e-010	0.547	0.0568	0.0182	0.00189

Persistence Time: 544 hr

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Reaction Time: 1.08e+003 hr  
Advection Time: 1.09e+003 hr  
Percent Reacted: 50.1  
Percent Advected: 49.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 209.7  
Water: 900  
Soil: 900  
Sediment: 3600  
Biowin estimate: 2.689 (weeks-months)

Advection Times (hr):

Air: 100  
Water: 1000  
Sediment: 5e+004

-----  
**Source** : Epona Associates, LLC  
**Test substance** : Chem Name : Benzenesulfonyl isocyanate, 4-methyl-  
Molecular Wt: 197.21  
**Reliability** : (2) valid with restrictions  
**Flag** : Critical study for SIDS endpoint  
05.04.2004

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#### 3.5 BIODEGRADATION

**Type** : anaerobic  
**Inoculum** : Pseudomonas sp. (Bacteria)  
**Contact time** :  
**Degradation** : (±) % after  
**Result** : other: low biodegradability  
**Deg. product** :  
**Method** :  
**Year** : 2001  
**GLP** : no data  
**Test substance** : other TS

**Remark** : PTSA reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3).

**Result** : A bacterium capable of utilising p-toluenesulphonamide was isolated from activated sludge. The isolated strain designated PTSA was identified as a Pseudomonas sp. using chemotaxonomic and genetic studies.  
Pseudomonas PTSA  
grew on p-toluenesulphonamide in a chemostat with approximately 90% release of sulphate and 80% release of ammonium. The isolate was also able to grow on 4-carboxybenzenesulphonamide and 3,4-dihydroxybenzoate but did not grow on p-toluenesulphonate. The transient appearance of 4-hydroxymethylbenzenesulphonamide and 4-carboxybenzenesulphonamide during p-toluenesulphonamide degradation proves oxidation of the methyl group is the initial attack in the biodegradation pathway. Both metabolites of p-toluenesulphonamide degradation were identified by high-performance liquid chromatography-mass spectrometry. 4-Carboxybenzenesulphonamide is probably converted into 3,4-dihydroxybenzoate and amidosulphurous acid.

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**Source**  
**Test substance**

The latter is a chemically unstable compound in aqueous solutions and immediately converted into sulphite and ammonium. Both sulphite and ammonium were formed during degradation of 4-carboxybenzenesulphonamide.

: Epona Associates, LLC  
: CAS Registry Number: 70-55-3  
Chemical Name: P-TOLUENESULFONAMIDE  
Synonyms: 4-METHYLBENZENESULFONAMIDE  
Molecular Formula: C7H9NO2S  
Molecular Weight: 171.22

**Reliability**  
**Flag**

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: (2) valid with restrictions  
: Critical study for SIDS endpoint

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## 4. Ecotoxicity

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### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :  
Species :  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : = 1314  
LC50 (14-day) : = 2005  
Method : other: estimated  
Year : 2004  
GLP : no  
Test substance : other TS

Remark : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). PTSI is not likely to be found in the environment.

Result : ECOSAR v0.99g Class(es) Found  
-----  
Neutral Organics

ECOSAR			Predicted	
Class	Organism	Duration	End Pt	mg/L
(ppm)				
=====				=====
Neutral Organic SAR: Fish	14-day	LC50	2005.498	
(Baseline Toxicity)				
Neutral Organics: Fish	96-hr	LC50	1314.445	

Source : Epona Associates, LLC  
Test condition : MOL FOR: C7 H9 N1 O2 S1  
MOL WT : 171.22  
Log Kow: 0.92 (KowWin estimate)  
Melt Pt:  
Wat Sol: 9619 mg/L (calculated)  
Test substance : SMILES : O=S(=O)(N)c(ccc(c1)C)c1  
CHEM : Benzenesulfonamide, 4-methyl-  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
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Type : flow through  
Species : Oncorhynchus mykiss (Fish, fresh water)  
Exposure period : 60 day(s)  
Unit : mg/l  
Effect Conc : = 9  
Method : other  
Year : 1996  
GLP : no data  
Test substance : other TS

Remark : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). PTSI is not likely to be found in the environment.

Result : Effect Endpoint Type:  
Effect Code (EFF) : GPHY - physiology, general  
Trend (TREND) : CHG - change  
Effect Category (EFFCAT): PHY - physiological: change in the organic processes or functions of an organism

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**Source** : Effect Tissue (TISSUE): BL - blood  
**Test condition** : Epona Associates, LLC  
: Age/Life Stage: ADULT, 206.5-670.7 G (grams)  
: Exposure Regimen: 60 (test duration); NR - not reported (minimum duration);  
: NR - not reported (maximum duration); Units: MI - minutes  
: Controls: M - multiple types of controls were reported by the author  
**Test substance** : CAS Registry Number: 70-55-3  
: Chemical Name: P-TOLUENESULFONAMIDE  
: Synonyms: 4-METHYLBENZENESULFONAMIDE  
: Molecular Formula: C7H9NO2S  
: Molecular Weight: 171.22  
**Reliability** : (2) valid with restrictions  
05.04.2004

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### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Type** : other  
**Species** : other: Daphnia  
**Exposure period** :  
**Unit** :  
**Method** : other: estimated  
**Year** : 2004  
**GLP** : no  
**Test substance** : other TS  
**Remark** : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). PTSI is not likely to be found in the environment.  
**Result** : ECOSAR v0.99g Class(es) Found  
-----  
Neutral Organics

	ECOSAR		Predicted	
	Class	Organism	Duration	End Pt mg/L (ppm)
	=====	=====	=====	=====
	Neutral Organics:	Daphnid	48-hr	LC50 1307.201
	Neutral Organics:	Daphnid	16-day	EC50 41.797

**Source** : Epona Associates, LLC  
**Test condition** : MOL FOR: C7 H9 N1 O2 S1  
: MOL WT : 171.22  
: Log Kow: 0.92 (KowWin estimate)  
: Melt Pt:  
: Wat Sol: 9619 mg/L (calculated)  
**Test substance** : SMILES : O=S(=O)(N)c(ccc(c1)C)c1  
: CHEM : Benzenesulfonamide, 4-methyl-  
**Reliability** : (2) valid with restrictions  
**Flag** : Critical study for SIDS endpoint  
12.04.2004

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### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : other algae: Green algae

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**Endpoint** :  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**EC50** : = 767  
**Method** : other: estimated  
**Year** : 2004  
**GLP** : no  
**Test substance** : other TS

**Remark** : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). PTSI is not likely to be found in the environment.

**Result** : ECOSAR v0.99g Class(es) Found

-----  
Neutral Organics

### ECOSAR

Class	Organism	Duration	End Pt	mg/L (ppm)
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=====

Neutral Organics:	Green Algae	96-hr	EC50	767.966
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Neutral Organics:	Green Algae	96-hr	ChV	41.140
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**Source** : Epona Associates, LLC

**Test condition** : MOL FOR: C7 H9 N1 O2 S1

MOL WT : 171.22

Log Kow: 0.92 (KowWin estimate)

Melt Pt:

Wat Sol: 9619 mg/L (calculated)

**Test substance**

: SMILES : O=S(=O)(N)c(ccc(c1)C)c1

CHEM : Benzenesulfonamide, 4-methyl-

**Reliability**

: (2) valid with restrictions

**Flag**

: Critical study for SIDS endpoint

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## 5.1.1 ACUTE ORAL TOXICITY

Type : LD50  
Value : = 2600 mg/kg bw  
Species :  
Strain :  
Sex :  
Number of animals :  
Vehicle :  
Doses :  
Method :  
Year : 2002  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Source : Epona Associates, LLC  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
09.06.2003

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## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.4 REPEATED DOSE TOXICITY

Type : Sub-acute  
Species : rat  
Sex : male/female  
Strain : other: Crj:CD(SD)  
Route of admin. : gavage  
Exposure period : 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)  
Frequency of treatm. : daily  
Post exposure period :  
Doses : 0, 120, 300, and 750 mg/kg  
Control group : yes  
Method : other: OECD 422  
Year : 1994  
GLP : yes  
Test substance : other TS  
  
Remark : PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3).  
  
Result : Dose-related hypersalivation was observed in all treatment groups. Significant decrease in body weight gains in the high-dose M relative to controls persisted throughout the dosing period. Relative kidney and liver weights were slightly increased in high-dose animals. A dose-dependent increase in white blood cells counts was observed in mid- and high-dose M and some F (1 low-, 12 mid-, and 7 high-dose groups). An increased number

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of neutrophils were observed in high-dose M. BUN, GOT, and chloride were significantly elevated in the two highest dose groups (M). GPT levels were significantly elevated and potassium levels decreased in the high-dose M. Four animals from the high-dose groups displayed hematuria within the first 3 d of dosing. There was an involution of the thymus in 8 high- and middosed F.

**Test condition** : Rat, Crj:CD(SD), adult, age n.p., 13 M and 13 F/dose Animals dosed orally (0, 120, 300, and 750 mg/kg [0, 0.701, 1.75, and 4.38 mmol/kg]) for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)

**Test substance** : p-TSA in 5% gum Arabic solution, >99.9% pure

**Reliability** : (1) valid without restriction

**Flag** : Critical study for SIDS endpoint

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### 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Bacterial reverse mutation assay

**System of testing** : S. typhimurium strains TA98, TA100, TA1535, TA1537; Escherichia coli WP2 ultra violet radiation A

**Test concentration** : 0, 312.5, 625, 1250, 2500, 5000 µg/plate [1.825, 3.65, 7.300, 14.60, and 29.20 µmol/plate]

**Cycotoxic concentr.** : 5000 ug/plate

**Metabolic activation** : with and without

**Result** : negative

**Method** :

**Year** : 1994

**GLP** : yes

**Test substance** : other TS

**Remark** : PTSl reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3).

**Result** : Mutagenic effects were not observed under the test conditions. Minimum toxic concentration observed for bacteria was 5000 µg/plate [29.20 µmol/plate] with and without activation.

**Source** : Epona Associates, LLC

**Test substance** : p-TSA in DMSO

**Reliability** : (1) valid without restriction

**Flag** : Critical study for SIDS endpoint

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**Type** : Chromosomal aberration test

**System of testing** : CHL cells

**Test concentration** : Without S9: 0, 0.33, 0.65, 1.30 mg/mL [0, 1.93, 3.80, 7.59 mM]; with S9: 0, 0.43, 0.85, 1.70 mg/mL [0, 2.5, 5.0, 9.9 mM].

**Cycotoxic concentr.** : >2.0 mg/mL [11.68 mM] with metabolic activation and 2.0 mg/mL [11.68 mM] without metabolic activation.

**Metabolic activation** : with and without

**Result** : negative

**Method** :

**Year** : 1994

**GLP** : yes

**Test substance** : other TS

**Remark** : PTSl reacts rapidly with excess water to form the corresponding carbamic

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<b>Result</b>	: acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (CAS number 70-55-3). : The test material was classified as "negative" for chromosomal aberrations, under the test conditions. The lowest concentration producing cell toxicity was >2.0 mg/mL [11.68 mM] with metabolic activation and 2.0 mg/mL [11.68 mM] without metabolic activation.
<b>Source</b>	: Epona Associates, LLC
<b>Test condition</b>	: Without S9: 0, 0.33, 0.65, 1.30 mg/mL [0, 1.93, 3.80, 7.59 mM]; with S9: 0, 0.43, 0.85, 1.70 mg/mL [0, 2.5, 5.0, 9.9 mM].
<b>Test substance</b>	: p-TSA in DMSO, purity 99.9%
<b>Reliability</b>	: (1) valid without restriction
<b>Flag</b>	: Critical study for SIDS endpoint
05.04.2004	(10)

### 5.6 GENETIC TOXICITY 'IN VIVO'

#### 5.8.1 TOXICITY TO FERTILITY

<b>Type</b>	: One generation study
<b>Species</b>	: rat
<b>Sex</b>	: male/female
<b>Strain</b>	: other: Crj:CD(SD)
<b>Route of admin.</b>	: gavage
<b>Exposure period</b>	: 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
<b>Frequency of treatm.</b>	: daily
<b>Premating exposure period</b>	
<b>Male</b>	: 42 days
<b>Female</b>	: 14 days
<b>Duration of test</b>	:
<b>No. of generation studies</b>	:
<b>Doses</b>	: 0, 120, 300, and 750 mg/kg
<b>Control group</b>	: yes
<b>NOAEL F1 offspring</b>	: = 300 mg/kg bw
<b>Method</b>	: OECD Guide-line 422
<b>Year</b>	: 1994
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS
<b>Result</b>	: In the high-dose group, newborns showed significant decrease in body weight and survival rate. Two of the high-dose female rats showed signs of difficult labor; all their offspring died by d 3 of lactation. NOAEL for F1 generation was 300 mg/kg [1.75 mmol/kg] under the test conditions.
<b>Source</b>	: Epona Associates, LLC
<b>Test condition</b>	: Rat, Crj:CD(SD), adult, 13 M and 13 F/dose Animals dosed orally (0, 120, 300, and 750 mg/kg [0, 0.701, 1.75, and 4.38 mmol/kg]) for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
<b>Test substance</b>	: p-TSA (99.9% pure)
<b>Reliability</b>	: (1) valid without restriction
<b>Flag</b>	: Critical study for SIDS endpoint
05.04.2004	(9)

## 5. Toxicity

Id 4083-64-1

Date 01.06.2004

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

<b>Species</b>	: rat
<b>Sex</b>	: male/female
<b>Strain</b>	: other: Crj:CD(SD)
<b>Route of admin.</b>	: gavage
<b>Exposure period</b>	: Animals dosed orally for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
<b>Frequency of treatm.</b>	: daily
<b>Duration of test</b>	:
<b>Doses</b>	: 0, 120, 300, and 750 mg/kg
<b>Control group</b>	: yes
<b>NOAEL teratogen.</b>	: = 300 - mg/kg bw
<b>Method</b>	: other: OECD 422
<b>Year</b>	: 1994
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS
<b>Result</b>	: Morphological observations for offspring revealed no teratogenic effect of the test substance. NOAEL for F1 generation was 300 mg/kg [1.75 mmol/kg] under the test conditions.
<b>Source</b>	: Epona Associates, LLC
<b>Test condition</b>	: Rat, Crj:CD(SD), Maternal doses: 0, 120, 300, 750 mg/kg/d [0, 0.701, 1.75, and 4.38 mmol/kg/d]
<b>Test substance</b>	: p-TSA (99.9% pure)
<b>Reliability</b>	: (1) valid without restriction
<b>Flag</b>	: Critical study for SIDS endpoint

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- (1) Atmospheric Oxidation (25 deg C) [AopWin v1.90]
- (3) ECOSAR Program (v0.99g)
- (4) HANSCH, C.; LEO, A.J. (1981) MEDCHEM PROJECT. ISSUE NO. 19, CLAREMONT, CA: POMONA COLLEGE, 1981; BiblioLine(c) 1997-2004, NISC International, Inc. All Rights Reserved.  
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- (5) HYDROWIN Program (v1.67)
- (6) Level III Fugacity Model (Full-Output)
- (7) Log Kow (WSKOW v1.40)
- (8) POWELL, M.D.; S.F. PERRY (1996). Respiratory and Acid-Base Disturbances in Rainbow Trout (*Oncorhynchus mykiss*) Blood During Exposure to Chloramine T, paratoluenesulphonamide, and.. Canadian Journal of Fisheries and Aquatic Sciences, 53(4): 701-708; 1996; BiblioLine(c) 1997-2004, NISC International, Inc. All Rights Reserved.  
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- (9) Unpublished report on Combined Repeat Dose and Reproductive Developmental Toxicity Screening Test of (Specific chemical)- HPV/SIDS test conducted by MHW; cited by OECD (1994); EMEA (1999) citChloramine-T [127-65-1] and Metabolite p-Toluenesulfonamide [70-55-3]  
Review of Toxicological Literature (2002) Prepared for  
Scott Masten, Ph.D. National Institute of Environmental Health Sciences P.O. Box 12233  
Research Triangle Park, North Carolina 27709 Contract No. N01-ES-65402  
Submitted by Karen E. Haneke, M.S. Integrated Laboratory Systems P.O. Box 13501  
Research Triangle Park, North Carolina 27709.
- (10) Unpublished report on Mutagenicity Test conducted by Ministry of Health and Welfare, Japan; cited by OECD (1994) ; cited in Chloramine-T [127-65-1] and Metabolite p-Toluenesulfonamide [70-55-3] Review of Toxicological Literature (2002) Prepared for Scott Masten, Ph.D. National Institute of Environmental Health Sciences P.O. Box 12233  
Research Triangle Park, North Carolina 27709 Contract No. N01-ES-65402 Submitted by Karen E. Haneke, M.S. Integrated Laboratory Systems P.O. Box 13501 Research Triangle Park, North Carolina 2
- (11) van Haperen, A M; van Velde, J W; van Ginkel, C G (2001) Akzo Nobel Chemicals Research Arnhem, Velperweg 76, 6824 BM, Arnhem, The Netherlands. F E M S Microbiology Letters, 204(2): pp. 299-304; 2001 Nov 13; BiblioLine(c) 1997-2004, NISC International, Inc. All Rights Reserved.  
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- (13) VanDeMark Inc., Material Data Safety Sheet, p-Toluenesufonyl Isocyanate. Doc: SE-0029-00 Rev. C 05/09/02.